### 1-(1-hydroxynaphthalen-2-yl)pentan-1-one 67013-64-3 | DTXSID00284025

## Model Performance

|        | n .    |
|--------|--------|
| Model  | I )ata |
| Widdei | Data   |
|        |        |

# Weighted KNN model

| 5-fold CV (75%) |      | Training (75 | Training (75%) |      | Test (25%) |  |
|-----------------|------|--------------|----------------|------|------------|--|
| Q2              | RMSE | R2           | RMSE           | R2   | RMSE       |  |
| 0.85            | 0.69 | 0.86         | 0.67           | 0.86 | 0.78       |  |

### Model Results

Predicted value: 3.36

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 6.86e-01

### Nearest Neighbors from the Training Set

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4-(Hex-1-en-1-yl)benzene-1,2-

diol

Measured: 3.82 Predicted: 3.41

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4-Phenylcyclohexanone

Measured: 2.30 Predicted: 2.55

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4-(1-naphthyloxy)butanoic acid

Measured: 3.50 Predicted: 3.11

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(4-cyclohexylphenoxy)acetic acid

Measured: 3.79 Predicted: 4.02